Universality and nonmonotonic finite-size effects above the upper critical dimension

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We analyze universal and nonuniversal finite-size effects of lattice systems in a L^d geometry above the upper critical dimension $d = 4$ within the O(n) symmetric φ^4 lattice theory. On the basis of exact results for $n \to \infty$ and one-loop results for $n = 1$ we identify significant lattice effects that cannot be explained by the φ^4 continuum theory. Our analysis resolves longstanding discrepancies between earlier asymptotic theories and Monte Carlo (MC) data for the five-dimensional Ising model of small size. We predict a *nonmonotonic* L dependence of the scaled susceptibility $\chi L^{-d/2}$ at T_c with a weak maximum that has not yet been detected by MC data.

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The concept of universality plays a fundamental role in statistical and elementary particle physics [1,2]. It implies that a unifying description of various physically different lattice and continuum systems near criticality can be given within the φ^4 field theory with the Hamiltonian

$$H = \int d^d x \left[\frac{r_0}{2} \, \varphi^2 + \frac{1}{2} (\nabla \varphi)^2 + u_0 \, (\varphi^2)^2 \right] . \tag{1}$$

The wide applicability of this theory is well established below the upper critical dimension $d^* = 4$ [1,2]. Particular accuracy has been achieved in testing the universal predictions of the φ^4 theory by means of numerical data for the universality class of the $d = 3$ Ising model not only for bulk properties but also for finite-size effects with periodic boundary conditions (p.b.c.) [3–5].

Less well established, however, is the range of applicability of the φ^4 theory for confined systems *above* the upper critical dimension where the critical exponents are mean-field like [1,2]. Early disagreements between Monte Carlo (MC) data for the finite $d = 5$ Ising model [6] and universal predictions based on H [4] have led to a longstanding debate [7]. New discrepancies between accurate MC data [8] and recent quantitative finite-size scaling predictions [9] based on the φ^4 lattice Hamiltonian

$$\hat{H} = \sum_i \left[\frac{r_0}{2} \varphi_i^2 + u_0 (\varphi_i^2)^2 \right] + \sum_{<ij>} \frac{J}{2} (\varphi_i - \varphi_j)^2 \tag{2}$$

have raised the question to what extent the φ^4 theory is capable of describing finite-size effects of the Ising model for $d > 4$. In particular the recently discovered [9,10] nonequivalence of H and $\hat{H}$ for finite systems is in striking contrast to the situation for $d < 4$. This non-equivalence may be relevant not only for higher-dimensional finite systems but also for three-dimensional physical systems for which mean-field theory provides a good description, such as systems with long but finite range interactions [11], polymer mixtures near their critical point of unmixing [12], and systems with a tricritical point [13].

In this Letter we resolve the existing discrepancies for $d > 4$ on the basis of exact results for the O(n) symmetric φ^4 theory in the limit $n \to \infty$ and of one-loop results for $n = 1$. Our analysis of both $\hat{H}$ and H with a smooth and a sharp cutoff is not restricted to large L and allows us to specify the range of validity of universal finite-size scaling for p.b.c. in a L^d geometry. We find, for p.b.c., that H with a smooth cutoff belongs to the same universality class as $\hat{H}$ whereas H with a sharp cutoff exhibits different nonuniversal finite-size effects. This implies that the lowest-mode prediction [4] of universal ratios at T_c for $d > 4$ is indeed valid asymptotically for both the lattice φ^4 theory and the continuum φ^4 theory with a smooth cutoff. We demonstrate, however, that the existing MC data for the $d = 5$ Ising model of small size [6–8] are outside the asymptotic scaling regime and cannot be explained by H because of significant lattice effects. We also demonstrate that our one-loop results based on $\hat{H}$ are in quantitative agreement with the MC data [8] for $4 \le L \le 22$ and that the one-loop two-variable scaling results [9,14] are well applicable to $L \gtrsim 12$, contrary to earlier conclusions [8,15]. We predict a weak maximum of the L-dependence of the scaled susceptibility $\chi L^{-d/2}$ at T_c which has not yet been detected in the MC data [8]. Our analysis implies $\xi_0 = 0.396$ for the bulk correlation-length amplitude of the $d = 5$ Ising model, in disagreement with $\xi_0 = 0.549$ found in Ref. [8].

We start from $\hat{H}$, Eq.(2), for the n-component variables φ_i on a finite sc lattice of volume L^d with a nearest-neighbor coupling $J > 0$. The basic question is to what extent $\hat{H}$ is equivalent to the spin Hamiltonian $H_s = -K \sum_{<ij>} s_i \, s_j$ where the n-component spin variables have a fixed length $s_i^2 = n$, in contrast to φ_i whose components $\varphi_{i\alpha}$ vary in the range $-\infty \le \varphi_{i\alpha} \le \infty$. For $n = 1, H_s$ is the Ising Hamiltonian with $s_i = \pm\, 1$ and $K > 0$.

An exact equivalence between $\hat{H}$ and H_s exists in the limit $u_0 \to \infty$, $r_0 \to -\infty$ at fixed $u_0/(Jr_0)$ for general L, n and d. Choosing $u_0/(Jr_0)$ such that $K = -Jr_0/(4u_0 n)$ we obtain by means of a saddle-point integration

$$\lim_{\substack{u_0 \to \infty \\ -r_0 \to \infty}} \chi = \frac{K}{J} \; \chi_s \tag{3}$$

where χ and χ_s are the susceptibilities

$$\chi = (nL^d)^{-1} \sum_{i,j} < \varphi_i \, \varphi_j > , \tag{4}$$

$$\chi_s = (nL^d)^{-1} \sum_{i,j} < s_i \, s_j > . \tag{5}$$

The weights in Eqs. (4) and (5) are $e^{-\hat{H}}$ and e^{-H_s}, respectively. For $n = 1$, this exact equivalence is of limited relevance since all calculations within the φ^4 model are performed at *finite* u_0. Hence, even in an exact theory, we have $\chi_s \neq J\chi/K$ at finite u_0. Therefore, in a quantitative comparison of χ with MC data for χ_s, one must allow for a (T and L independent) overall amplitude A which is adjusted such that $\chi_s = AJ\chi/K$. For finite u_0, the constant A accounts for an appropriate normalization of the variables φ_i relative to the discrete variables $s_i = \pm 1$. In an approximate theory, the value of A depends on the approximations made for χ. This corresponds to an adjustment merely of the *nonuniversal bulk* amplitude and not of the L dependence of χ (for $d = 3$ see, e.g., Ref. [5]). An adjustment of A was not taken into account in the analysis of Ref. [8].

Of particular interest is the case $n \to \infty$ since it provides the opportunity of studying the *exact* u_0 dependence including $u_0 \to \infty$. This reveals the structural similarity between χ at finite u_0 and at $u_0 = \infty$. This is most informative for $d > 4$ where the leading and subleading powers of L are independent of n and should apply also to the Ising universality class with $n = 1$.

For $n \to \infty$ at fixed $u_0 n$ the susceptibility $\hat{\chi} = 2J\chi$ for p.b.c. is determined implicitly by [10]

$$\hat{\chi}^{-1} = \; r_0/(2J) \; + \; J^{-2} u_0 n \; L^{-d} \sum_{\mathbf{k}} G_{\mathbf{k}}(\hat{\chi}^{-1}), \tag{6}$$

with $G_{\mathbf{k}}(\hat{\chi}^{-1}) = (\hat{\chi}^{-1} + J_{\mathbf{k}})^{-1}$ and $J_{\mathbf{k}} = 2\sum_{j=1}^{d}(1 - \cos k_j)$ where $\sum_{\mathbf{k}}$ runs over $\mathbf{k}$ vectors with components $k_j = 2\pi m_j/L, \;\; m_j = 0, \pm 1, \pm 2..., j = 1, 2, ..., d$ in the range $-\pi \leq k_j < \pi$. At $T = T_c$ we derive from Eq. (6) the exact implicit equation for $d > 4$

$$\hat{\chi}^2 = L^d \;\; \frac{\lambda_0(u_0) - \hat{\chi}^{(4-d)/2} \; f_b \; (\hat{\chi}^{-1})}{1 - L^d \;\; \hat{\chi}^{-1} \; \hat{\Delta}_1(\hat{\chi}^{-1}, \; L)} \tag{7}$$

with $\lambda_0(u_0) = \; (J^2 + u_0 n \int_{\mathbf{k}} J_{\mathbf{k}}^{-2}) \; (u_0 n)^{-1}$ and

$$f_b(\hat{\chi}^{-1}) = \hat{\chi}^{(d-6)/2} \int_{\mathbf{k}} \left[J_{\mathbf{k}}^2 (\hat{\chi}^{-1} + J_{\mathbf{k}}) \right]^{-1} , \tag{8}$$

$$\hat{\Delta}_m(\hat{\chi}^{-1}, L) = \int_{\mathbf{k}} G_{\mathbf{k}}(\hat{\chi}^{-1})^m - L^{-d} \sum_{\mathbf{k} \neq \mathbf{0}} G_{\mathbf{k}}(\hat{\chi}^{-1})^m, \tag{9}$$

where $\int_{\mathbf{k}} \equiv (2\pi)^{-d} \int d^d \; k$ with $|k_j| \leq \pi$. We see that the structure of the L dependence of $\hat{\chi}$ for finite $u_0 > 0$ is the same as for $u_0 \to \infty$ where $\lambda_0(u_0)$ is reduced to $\lambda_0 = \int_{\mathbf{k}} J_{\mathbf{k}}^{-2}$. It is reasonable to expect that also for $n = 1$ the calculation of $\hat{\chi}$ at finite u_0 yields essentially the correct structure of χ_s.

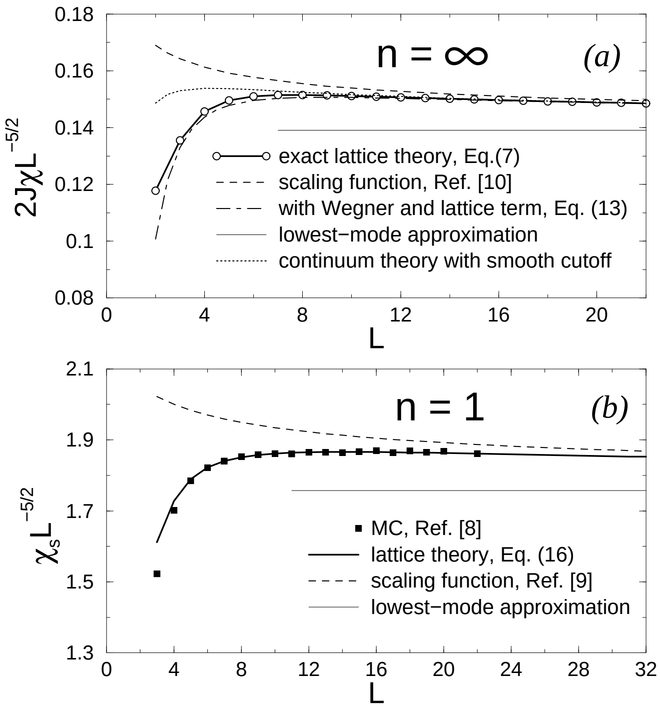

FIG. 1. Scaled susceptibilities for $d = 5$ at T_c. Solid and dashed lines approach the lowest-mode lines for $L \to \infty$.

In Fig. 1a we show the exact result of $\hat{\chi} L^{-5/2}$ for $n \to \infty$ and $d = 5$ at T_c by solving Eq. (7) numerically with $\lambda_0 = \int_{\mathbf{k}} J_{\mathbf{k}}^{-2} = 0.01935$. We find that $\hat{\chi} L^{-5/2}$ has a weak maximum at $L = 9$ which is not contained in the (large L) scaling form $\hat{\chi}_{scal} = L^{d/2} \; \tilde{P}(L^{4-d}/\lambda_0)$ of Ref. [10] (dashed curve). In $\hat{\chi}_{scal}$ the nonasymptotic Wegner correction $\propto f_b$ was neglected and $\hat{\Delta}_1$ was approximated only by the leading term $\hat{\Delta}_1 = I_1(\hat{\chi}^{-1} \; L^2) \; L^{2-d}$ with

$$I_m(x) = \int_0^\infty dt \;\; \frac{t^{m-1}[K_b(t)^d - K(t)^d + 1]}{(2\pi)^{2m} e^{(xt/4\pi^2)}}, \tag{10}$$

where $K_b(t) = (\pi/t)^{1/2}$ and $K(t) = \sum_{j=-\infty}^{\infty} \exp(-j^2 t)$. Both $\hat{\chi}$ and $\hat{\chi}_{scal}$ show the predicted [9] slow $O(L^{(4-d)/2})$ approach to the large-L limit $\hat{\chi}_0 L^{-d/2} = \lambda_0^{1/2}$ corresponding to the lowest-mode approximation (horizontal line in Fig. 1a). Note that both $\hat{\chi}$ and $\hat{\chi}_{scal}$ approach $\hat{\chi}_0$ from *above*.

The small difference between $\hat{\chi}$ and $\hat{\chi}_{scal}$ in Fig. 1a for $L \gtrsim 15$ arises from the negative Wegner correction term $-\hat{\chi}^{(4-d)/2} f_b(\hat{\chi}^{-1}) \propto -L^{(4-d)d/4} f_b(0)$ in the numerator of Eq. (7). The pronounced departure of $\hat{\chi}$ from $\hat{\chi}_{scal}$ for $L \lesssim 10$, however, is a lattice effect that is dominated by the subleading term $-\hat{M}_1 L^{-d}$ in

$$\hat{\Delta}_1(\hat{\chi}^{-1}, L) = I_1(x) L^{2-d} - \hat{M}_1(x) L^{-d} + O(L^{-d-2}), \tag{11}$$

$$\hat{M}_1(x) = \int_0^\infty dt\; \frac{[K(t)^{d-1}K''(t) - K_b(t)^{d-1}K_b''(t)]}{e^{(xt/4\pi^2)}}, \quad (12)$$

with $x = \hat{\chi}^{-1}L^2$. Unlike the leading term $I_1 L^{2-d}$, the lattice term $-\hat{M}_1 L^{-d}$ cannot be incorporated in the universal finite-size scaling function $\tilde{P}(y)$ which depends on $y = (L/l_0)^{4-d}$ with $l_0^{4-d} = \lambda_0$. In summary, the leading L dependence of $\hat{\chi}$ is represented as

$$\hat{\chi} = \left(\lambda_0 L^d \frac{1 \;-\; q_2 L^{(4-d)d/4}}{1 - q_1 L^{(4-d)/2} + q_3 L^{-d/2}}\right)^{1/2} \quad (13)$$

where $q_1 = \lambda_0^{-1/2} I_1(x)$, $q_2 = \lambda_0^{-d/4}\; f_b(0)$, and $q_3 = \lambda_0^{-1/2}\hat{M}_1(x)$. The functions $I_1(x)$ and $\hat{M}_1(x)$ have a weak x dependence with $I_1(0) = 0.107$ and $\hat{M}_1(0) = 0.676$ for $d = 5$. Eq. (13) is shown in Fig. 1a as dot-dashed line which approximates the exact result, Eq. (7), with very good accuracy down to $L = 3$.

Now we turn to the question to what extent H, Eq. (1), is equivalent to $\hat{H}$. From our result of $\hat{\chi}$, Eqs. (6) - (9), we obtain the corresponding result of $\chi_{field} = n^{-1}\int d^d x < \varphi(x)\varphi(0) >$ after replacing $J_{\mathbf{k}}$ by k^2 and setting $2J = 1$. A novel feature for $d > 4$ is the fact that Δ_1 depends significantly on the cutoff procedure. We need to distinguish two cases : (a) a *sharp* cutoff Λ which restricts the $\mathbf{k}$ vector to $|k_j| \le \Lambda$, (b) a *smooth* cutoff Λ where $-\infty \le k_j \le \infty$ but where $(\hat{\chi}^{-1} + k^2)^{-m}$ is replaced by the (Schwinger type) regularized form [2] $(\hat{\chi}^{-1}+k^2)^{-m}_{reg} = \int_{\Lambda^{-2}}^\infty ds\; s^{m-1}\; \exp\,[-(\hat{\chi}^{-1} + k^2)s]$. The former case (a) implies [9,10] $\Delta_1 \propto L^{-2}$ and $\chi_{field} \propto L^{d-2}$ at T_c which differs fundamentally from the lattice result $\hat{\chi} \propto L^{d/2}$. In the latter case (b), however, Eqs. (11) and (12) are replaced by

$$\Delta_1(\hat{\chi}^{-1}, L) = I_1(x)L^{2-d} - M_1(\hat{\chi}^{-1})L^{-d} + O(e^{-\Lambda^2 L^2}), \quad (14)$$

$$M_1(\hat{\chi}^{-1}) = \hat{\chi}[1 - \exp(-\hat{\chi}^{-1}\Lambda^{-2})], \quad (15)$$

with the same leading term $I_1 L^{2-d}$. This implies that χ_{field} with a smooth cutoff has the same asymptotic (large L) finite-size scaling behavior as $\hat{\chi}_{scal}$. Adjustment of the leading amplitude $\lambda_0^{field} = \int_{\mathbf{k}}(k^{-2})^{-2}_{reg}$ to the lattice counterpart $\lambda_0 = \int_{\mathbf{k}} J_{\mathbf{k}}^{-2}$ fixes the cutoff as $\Lambda = 0.185$ and $M_1(0) = \Lambda^{-2} = 0.034$ for $d = 5$ which is smaller than $\hat{M}_1(0)$ by a factor of 20. This difference between $\hat{M}_1$ and M_1 constitutes a significant lattice effect for small L that is exhibited in Fig. 1a, with $\chi_{field}\; L^{-5/2}$ represented by the dotted line. We conclude that H with a *smooth* cutoff yields the same (large L) finite-size scaling behavior as $\hat{H}$ (for cubic geometry and p.b.c.) but does not account for the strong L-dependence of $\hat{\chi}L^{-d/2}$ for small L. We expect this conclusion to hold for general n.

Now we consider $\hat{H}$ for the relevant case $n = 1$. We start from the one-loop result for $\hat{\chi} = 2J\chi$ and for the ratio $Q = < \Phi^2 >^2 \,/\, < \Phi^4 >$ of moments $< \Phi^m >$ for the order parameter distribution where $\Phi = L^{-d}\,\Sigma_j\,\varphi_j$. The analytic result reads for arbitrary L [9]

$$\hat{\chi} = L^{d/2}\,(u_0^{eff})^{-1/2}\,\vartheta_2\,(Y^{eff}), \quad (16)$$

$$Q = \vartheta_2(Y^{eff})^2 \,/\, \vartheta_4(Y^{eff}), \quad (17)$$

$$Y^{eff} = L^{d/2}\, r_0^{eff}(u_0^{eff})^{-1/2}, \quad (18)$$

$$\vartheta_m(Y) = \frac{\int_0^\infty ds s^m \exp\left(-\frac{1}{2}Ys^2 - s^4\right)}{\int_0^\infty ds \exp\left(-\frac{1}{2}Ys^2 - s^4\right)} \quad (19)$$

with the effective parameters

$$r_0^{eff} = \tilde{a}_0 t + 12\tilde{u}_0(S_1 - \lambda_0) + 144\;\tilde{u}_0^2 M_0^2 S_2, \quad (20)$$

$$u_0^{eff} = \tilde{u}_0 - 36\tilde{u}_0^2 S_2, \quad (21)$$

$$S_m = L^{-d}\sum_{\mathbf{k}\neq\mathbf{0}}(\tilde{a}_0 t + 12\tilde{u}_0 M_0^2 + J_{\mathbf{k}})^{-m}, \quad (22)$$

$$M_0^2 = (L^d\;\tilde{u}_0)^{-1/2}\;\vartheta_2(L^{d/2}\;\tilde{a}_0 t\;\tilde{u}_0^{-1/2})\,. \quad (23)$$

The r.h.s. of Eqs. (16) - (23) depend only on the parameters $\tilde{u}_0 = u_0/(4J^2)$ and $\tilde{a}_0 = a_0/(2J)$ where $a_0 = (r_0 - r_{0c})/t$ with $t = (T - T_c)/T_c$. Eqs. (16) - (23) were evaluated previously [9] only for large L. Here we present the numerical evaluation of Eqs. (16) - (23) for arbitrary $L \le 32$ *without further approximation* for $d = 5$ including Wegner corrections and lattice terms. Our strategy of adjusting $\tilde{u}_0$ is based on the fact that Q at $T = T_c$ depends only on $\tilde{u}_0$ and that no overall adjustment for Q is required since $\lim_{L\to\infty} Q = Q_0$ is universal. Thus we adjust $\tilde{u}_0 = 0.93$ to the MC data [8] of Q at T_c (Fig. 2), then we use the same $\tilde{u}_0$ for $\hat{\chi}$ at T_c. For the comparison of $\hat{\chi}$ with the MC data for χ_s at T_c we introduce the amplitude A according to $\chi_s = AJ\chi/K = A\hat{\chi}/(2K_c)$. Using [8] $K_c = 0.1139155$ and adjusting $A = 0.678$ yields the solid line in Fig. 1b. At $T \neq T_c$ we determine $\tilde{a}_0 = 2.87$ from the *bulk* susceptibility $\chi_s = 1.322t^{-1}$ of series expansion results [16].

In Figs. 1b-3 our analytic result (solid lines) is compared with the MC data of Ref. [8]. We conclude that our one-loop finite-size theory based on $\hat{H}$ satisfactorily describes the existing MC data for $4 \le L \le 22$, both at T_c and away from T_c (Fig.3). We attribute the remaining deviations of Q for small L to the (expected) inaccuracy of our one-loop approximation. At $T = T_c$ our analytic results approach the lowest-mode results $\lim_{L\to\infty}\chi_s L^{-5/2} = p_0 = 1.757$ and $Q_0 = 0.4569$ (horizontal lines in Figs. 1b and 2) from *above*, in particular our theory predicts a (weak) maximum of $\chi_s L^{-5/2}$ at T_c (similar to that in Fig. 1a for $n = \infty$) that has not yet been detected in the MC data [8]. Our theory also predicts a nonmonotonic L dependence of Q at T_c (Fig. 2) and of the scaled magnetization $< |\Phi| > L^{5/4}$ at T_c.

Finally we answer the question to what extent the MC data in Figs. 1b-3 can be described by the finite-size scaling forms of $\hat{\chi}_{scal} = 2J\chi_{scal}$ and Q_{scal} derived previously (Eqs. (76) - (88) of Ref. [9]) on the basis of $\hat{H}$. These scaling forms neglect Wegner corrections and lattice effects. We have found that the same scaling functions can be derived on the basis of H provided that a

smooth cutoff is used. The corresponding scaling functions depend on the two scaling variables $x = t(L/\xi_0)^2$ and $y = (L/l_0)^{4-d}$ where $\xi_0 \propto \tilde{a}_0^{-1/2}$ is the amplitude of the bulk correlation length and $l_0 \propto \tilde{u}_0^{1/(d-4)}$ is a second reference length. Thus, instead of $\tilde{u}_0$ and $\tilde{a}_0$, we now have l_0 and ξ_0 as adjustable parameters. Since the one-loop results for $\hat{\chi}$ and $\hat{\chi}_{scal}$ differ at $O(\tilde{u}_0^2)$ one must allow for a different amplitude $A_{scal} \neq A$ in the adjustment of $\hat{\chi}_{scal}$ to χ_s. Using the same strategy of adjustment as described above we find $l_0 = 2.641$ from Q at T_c and $A_{scal} = 1.925$ from $\chi_s = A_{scal}\hat{\chi}_{scal}/(2K_c)$. Finally we determine $\xi_0 = 0.396$ from the one-loop bulk result $\lim_{t\to 0}\lim_{L\to\infty}\chi_s t = A_{scal}\xi_0^2/(2K_c) = 1.322$. The corresponding scaling results are shown in Figs. 1b-3 as dashed lines. We identify the significant departure of the MC data for χ_s at T_c from the dashed line for $L \lesssim 12$ as a lattice effect that is well described by our full one-loop theory (solid line in Fig. 1b) but which is not captured by the scaling form.

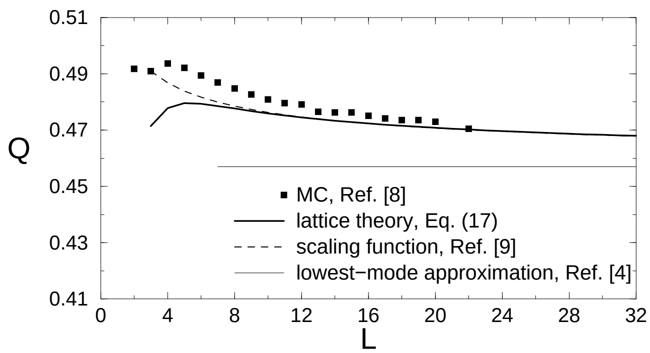

FIG. 2. Moment ratio Q at T_c for $d = 5$ and $n = 1$. Solid and dashed lines approach the lowest-mode line for $L \to \infty$.

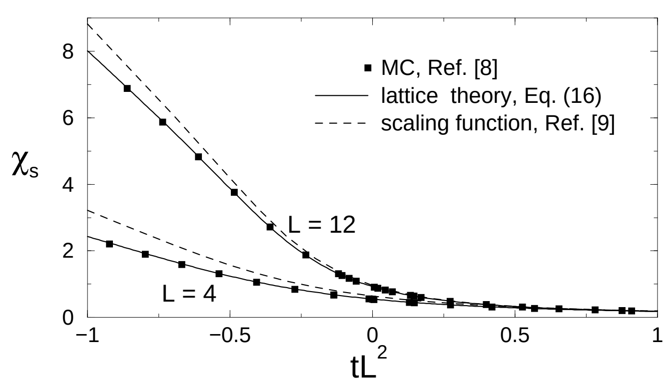

FIG. 3. Temperature dependence of susceptibilities for $d = 5$ and $n = 1$: $10^{-2}\chi_s$ for $L = 4$ and $10^{-3}\chi_s$ for $L = 12$.

This failure of the scaling form for $L \lesssim 12$ was first observed by Luijten et al. [8]. We see, however, that there is good agreement of our scaling results with the MC data for $L \gtrsim 12$, contrary to the disagreement found in Ref. [8]. The latter disagreement is due to the (unjustified) identification [8] $J = K, \chi_s = \chi$ corresponding to $A_{scal} = 1$ which, together with the fitting formula Eq.(32) of Ref. [8], implied $\xi_0 = 0.549$ and $l_0 = 0.603$. This formula omits the leading Wegner correction $\propto L^{(4-d)d/4}$ and a negative lattice term $\propto L^{-d/2}$ [compare our Eq.(13)] and therefore implies an *increasing* $\chi_s L^{-5/2}$ (Fig. 9 of Ref. [8]) towards $\lim_{L\to\infty}\chi_s L^{-5/2} = p_0 = 1.91$, in contrast to the *decreasing* $\chi_s L^{-5/2}$ with $p_0 = 1.76$ of our one-loop theory. More accurate MC data would be desirable which could distinguish between our quantitative predictions in Figs. 1b and 2 and those implied by the analysis of Ref. [8]. It would also be desirable to determine ξ_0 for the $d = 5$ Ising model (e.g. from series expansion results) in order to resolve the disagreement between our prediction for ξ_0 and that of Ref. [8].

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